MODEL OF BIOACCUMULATOR

1. Modelling

As the Phitoquelatin is expressed linked with Omp-A we can treat it like a single complex C. So we have the reaction scheme

- $\xrightarrow{k_C} C \xrightarrow{\delta_C}$
- $C + M \underset{k_-}{\overset{k_+}{\rightleftharpoons}} C^*$

Where M is the free mercury and C^* is the mercury linked with the complex C, k_C is the rate of production of the complex and δ_C is the rate of degradation of the complex.

I will note $[C]$ as the amount of the complex per cell, $[C^*]$ as the amount of the complex linked with mercury per cell and $[M]$ to the concentration of mercury, pay attention to the units.

The equation for the reactions are

$$\frac{d[C]}{dt} = k_C - \delta_C[C] - [C][M]k_+ + k_-[C^*] \tag{1}$$

$$\frac{d[C^*]}{dt} = [C][M]k_+ - [C^*]k_- \tag{2}$$

Also as the total concentration of mercury does not change we have that $M_0 = [M] + \frac{n}{N_{Av}}[C^*]$ where $[M]$ is the concentration of free mercury , n is the amount of cells and N_{Av} is the Avogadro's number to convert units, this last thing is for the units conversion.

$$\frac{d[C]}{dt} = k_C - \delta_C[C] - [C](M_0 - \frac{n}{N_{Av}}[C^*])k_+ + [C]k_- \tag{3}$$

$$\frac{d[C^*]}{dt} = [C](M_0 - \frac{n}{N_{Av}}[C^*])k_+ - [C^*]k_- \tag{4}$$

We can assume that the rate of splitting of the complex C^* is 0, because Mercury and Phitoquelatin have very hight affinity and the degradation of the complex is very slow then $\delta_C = 0$

$$\frac{d[C]}{dt} = k_C - [C](M_0 - \frac{n}{N_{Av}}[C^*])k_+ \tag{5}$$

the interpretation of the variation of C is simple, k_C is the production term and the other thing is the consumption due to mercury binding.

$$\frac{d[C^*]}{dt} = [C](M_0 - \frac{n}{N_{Av}}[C^*])k_+ \tag{6}$$

If we are at estacionaria time phase we have that the amount of cells is n, is constant, then we can say that the amount of free mercury will change as

$$M(t) = M_0 - \frac{n}{N_{Av}}[C^*] \tag{7}$$

If we are considering the exponential phase then, since bacteria grow exponentially, it is often useful to plot the logarithm of the relative population size $[Y = ln(N/N_0)]$ against time .So lets use the Gompertz equation to model this.

The three phases of the growth curve can be described by three parameters: the maximum specific growth rate, μ_m is defined as the tangent in the inflection point; the lag time, λ, is defined as the x-axis intercept of this tangent; and the asymptote $[A = ln(N/N_0)]$ is the maximal value reached. Here we are not considering the death rate. [**?**]

$$Y(t) = Ae^{-e^{\frac{\mu_m e}{A}(\lambda - t)+1}} \tag{8}$$

then the equations will look like

$$\frac{d[C]}{dt} = k_C - [C](M_0 - \frac{e^{Y(t)}N_0}{N_{Av}}[C^*])k_+ \tag{9}$$

$$\frac{d[C^*]}{dt} = [C](M_0 - \frac{e^{Y(t)}N_0}{N_{Av}}[C^*])k_+ \tag{10}$$

where N_0 is the inial cell amount,then the amount of mercury in function of time is

$$M(t) = M_0 - \frac{e^{Y(t)}N_0}{N_{Av}}[C^*] \tag{11}$$